

# X-ray microdiffraction applications in integrated circuits

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# X-ray Microbeam Instruments

- Microbeam facilities exist in all major synchrotrons.
- Used for:
  - Metrology,
  - Failure analysis,
  - Applied Science.
    - Provide boundary conditions for formulations.
    - Provide test data.

# SPRing-8 (Super Photon ring-8 GeV)

Industrial Consortium ID (13 companies)	BL16 XU	Undulator	4.5 - 40 keV	X-ray diffraction, X-ray fluorescence analysis and X-ray microbeam analysis for characterization of new industrial materials.
Industrial Consortium BM (13 companies)	BL16 B2	Bending Magnet	3.5 - 60 keV	XAFS and X-ray topography for characterization of new industrial materials.
Hyogo (Hyogo Prefecture)	BL24 XU	Undulator	3.5 - 60 keV	Protein crystal structure analysis. Surface/interface analysis of inorganic materials. X-ray microbeam analysis. X-ray imaging.



# ESRF

- **μ-FID-22 :Micro-Fluorescence, Imaging and Diffraction,**
  - Phase-contrast imaging
  - Phase-contrast microtomography
  - Micro-topography
  - Holography and interferometry
- ID19 - Topography & Tomography Beamline
- Microfocus beamline ID13
  - Diffraction
  - Small angle x-ray scattering
  - Scanning x-ray microfluorescence

# APS

## Sector 2: X-ray Microscopy Group

- 2-ID-D : High-resolution fluorescence and diffraction imaging
- 2-ID-E: Sub-micron x-ray fluorescence mapping
- 2-ID-B: High-resolution imaging, coherent scattering.
- MHATT-CAT-Sector7 /UNICAT Beamline 34:
  - Grain by grain strain/texture mapping.
  - Depth resolved mapping.

X-ray nanoprobe beamline; Under development.

# Microscopes at the ALS

- 1.4.3** IR Spectromicroscopy
- 4.0.1-2** Photoemission Electron Microscopy
- 5.3.2** Scanning Transmission X-Ray Microscopy for Polymers
- 6.1.2** Imaging X-Ray Microscopy
- 6.3.1** MicroESCA
- 7.0.1** Scanning Photoemission Microscopy, Scanning Transmission X-Ray Microscopy
- 7.3.1.1** Photoemission Electron Microscopy
- 7.3.1.2** MicroXPS
- 7.3.3** Micro X-Ray Diffraction
- 10.3.1** X-Ray Fluorescence Microprobe
- 10.3.2** MicroXAS
- 11.3.2** EUV Lithography Mask Inspection



## ➤CHESS

- B2 bend magnet station,
- Tapered capillary optic, Smallest beam: 1000 Å diameter @ 6 keV.
- $10^6$  photons/sec at the sample @ 12.3 keV
- Microstructure evaluation (Laue photos).

## ➤NSLS

- X20-IBM
- X13-B Under construction.

- There are quite exciting machines that are doing microbeam x-ray analysis.
- This is a hot area:
  - ESRF now reports microbeam results as a separate category.
- All have advantages and limitations.
  - Ease of access,
  - Multiple techniques with minimal set-up.
- New rings are being designed with microspot beamlines.



# IBM Microdiffraction program

- We are currently investigating:
  - The basic theory of stress/strain analysis in single crystals.
  - Diffraction from strained crystallites.
  - X-ray information volumes.
  - X-ray microbeam metrology.

### Stresses affect device behavior:

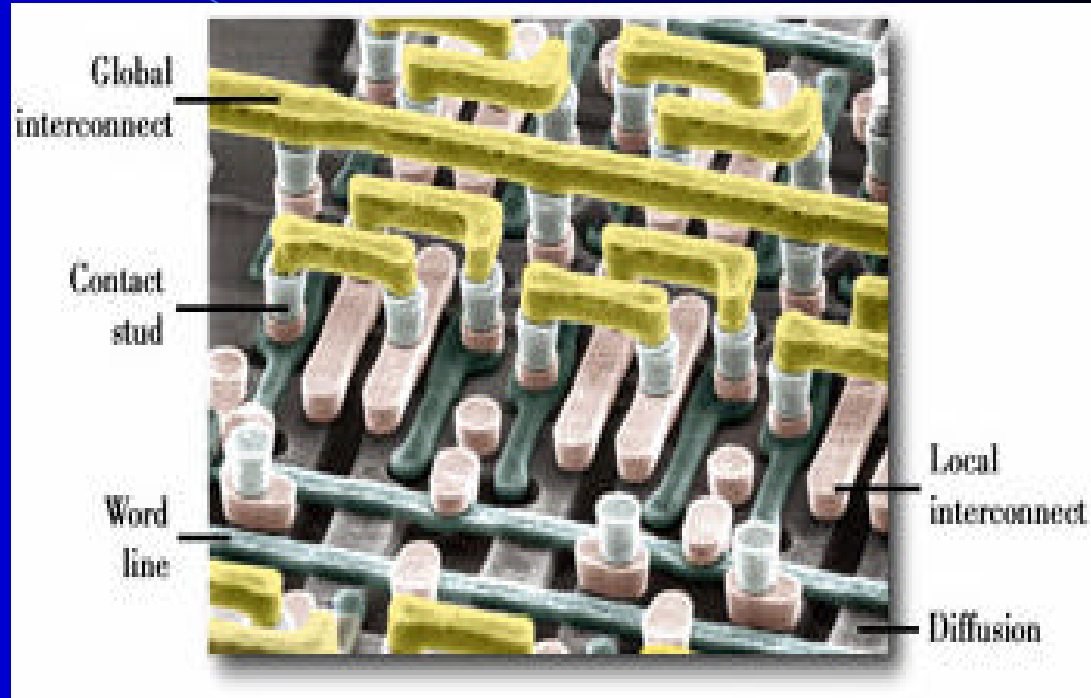
- reliability concerns
- performance issues
  - Faster devices.

### Aspects of controlling strain:

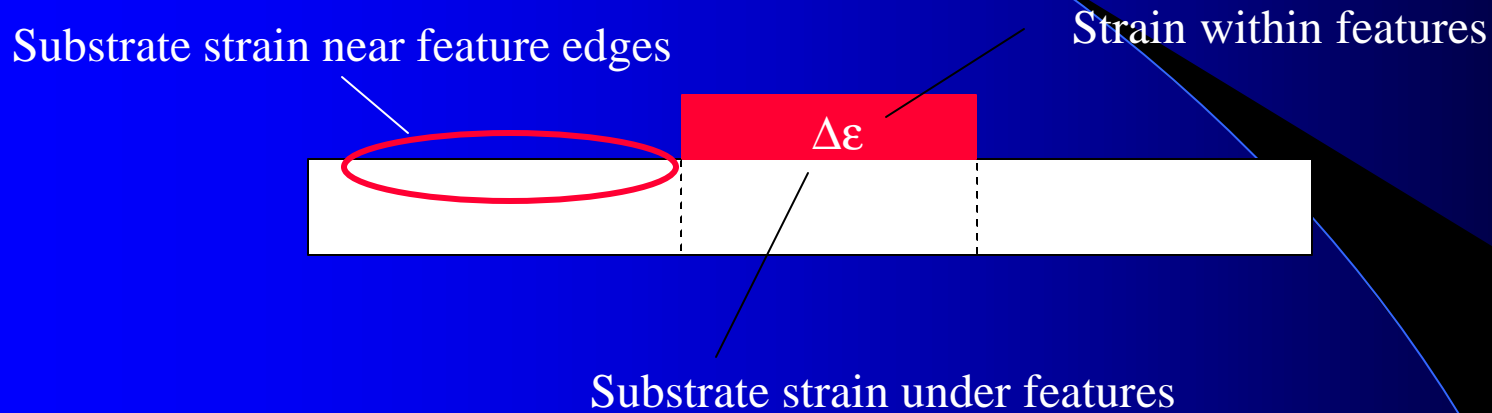
- stresses during fabrication
- feature geometry and density
- interfacial integrity

### Modeling of mechanical behavior:

- constitutive equations based on bulk behavior
- edge effects dominate stress / strain evolution
- experimental verification is necessary



# Detection of strain by x-ray diffraction



Synchrotron-based x-ray scanning topography:

- dynamic to kinematic transition in substrate diffracted intensity
- highly sensitive to minute strain gradients in single crystal substrates

# Measurements

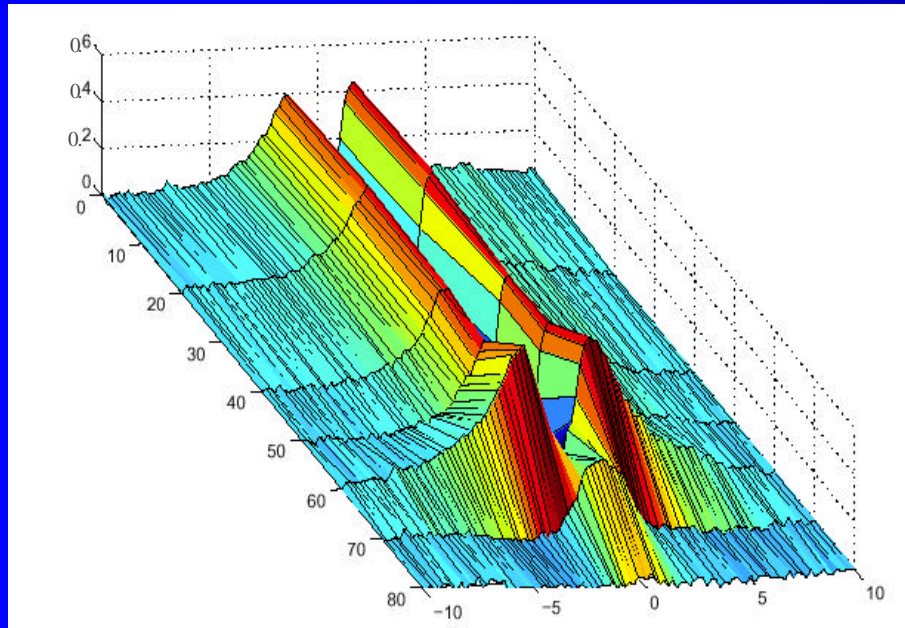
Conducted at APS 2ID-D

- UHV/CVD 0.24  $\mu\text{m}$  thick  $\text{Si}_{0.86}\text{Ge}_{0.14}$  on Si (001)
- 100  $\mu\text{m}$  features etched (various widths)
- Fresnel zone plate optics, beam size  $\sim 0.3 \mu\text{m}$
- $E = 9.2 \text{ keV}$
- Map Si (004) and SiGe (004) diffracted intensity

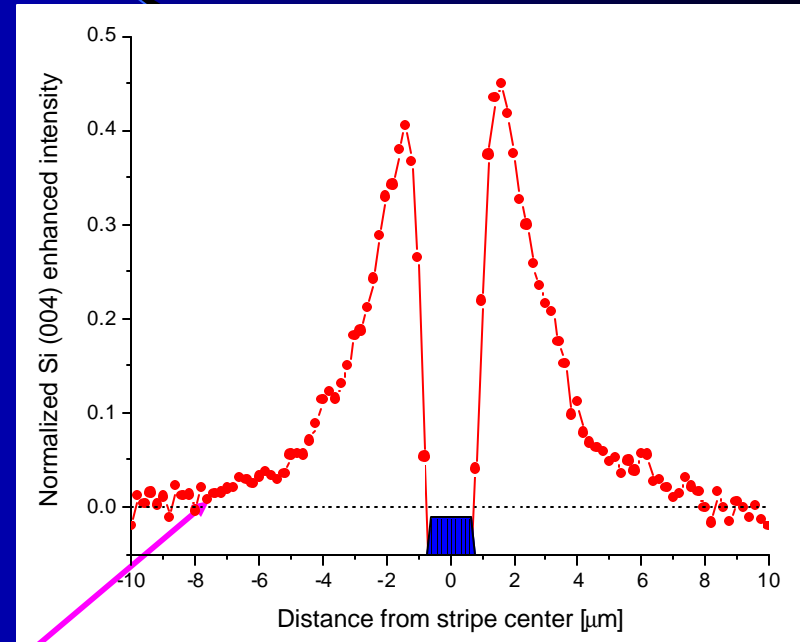


# Experimental: 1.5 $\mu\text{m}$ SiGe feature on Si (001)

Normalized Si diffracted intensity  $[\Delta I/I_0]$



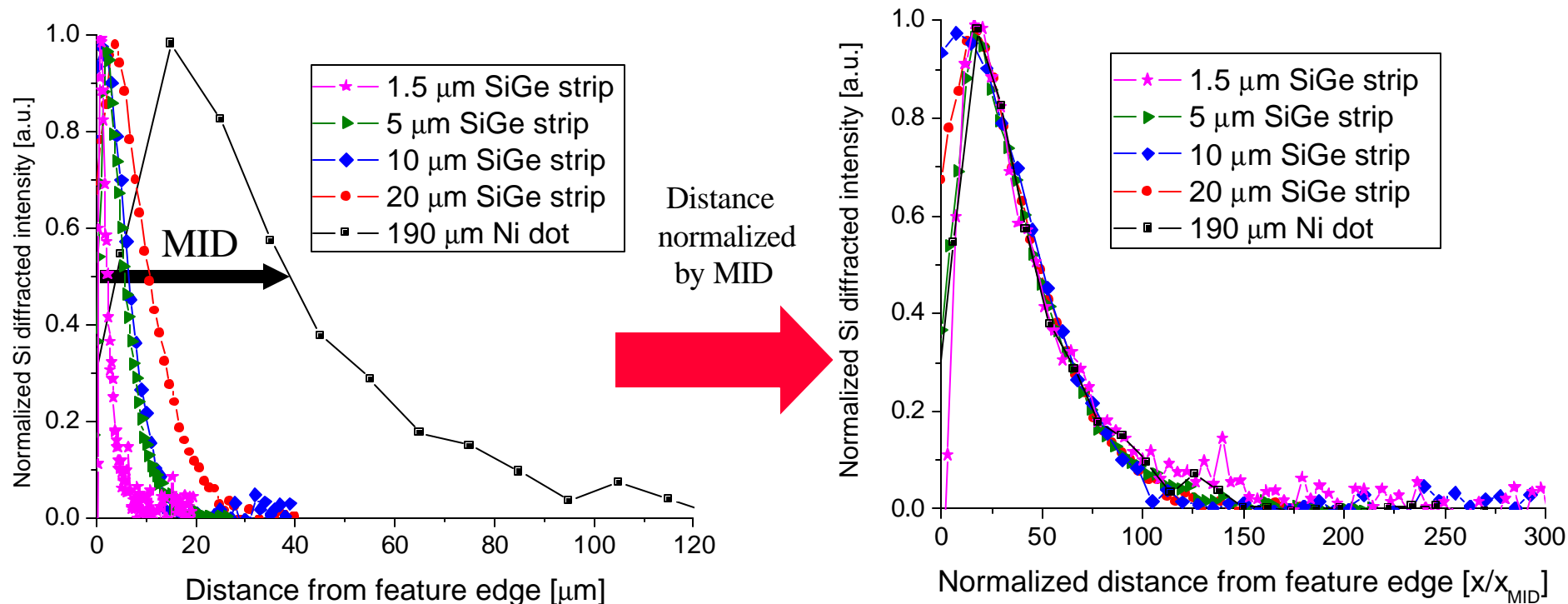
Distance from stripe center [ $\mu\text{m}$ ]



- Distortion in Si substrate detected  $\sim 7 \mu\text{m}$  away from stripe edge (30 x/t)
  - The smaller the beam size, the better the resolution.
  - The 0.3 micron beam size is very important.

# Comparison of distortion fields in Si

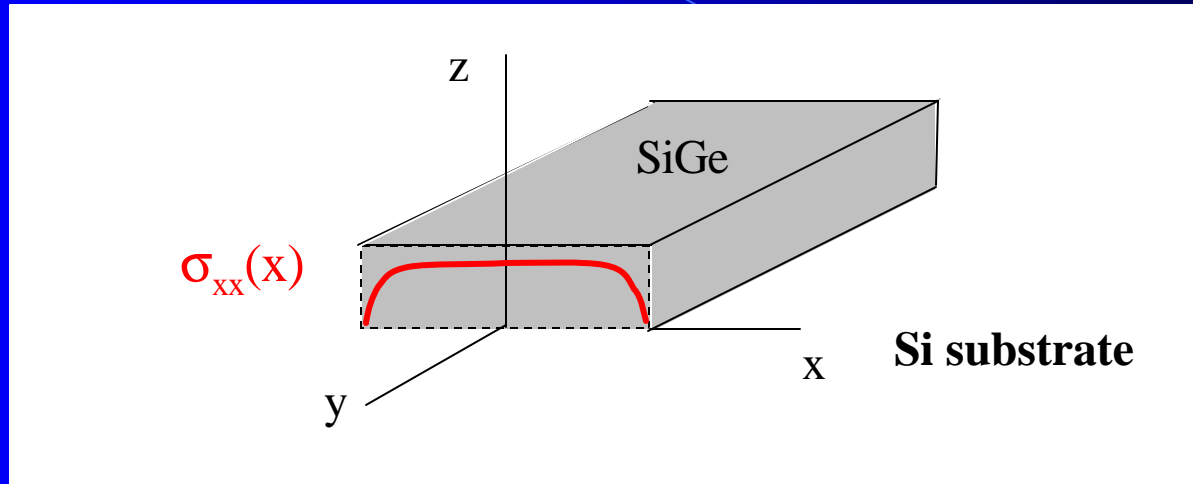
- Extent of deformation in Si: 7  $\mu\text{m}$  to 30  $\mu\text{m}$  from SiGe feature edge



Decay of magnitude of strain follows characteristic curve:

➤ NOT predicted by traditional mechanical models (analytical, FEM)

# Elastic relaxation due to edge effects



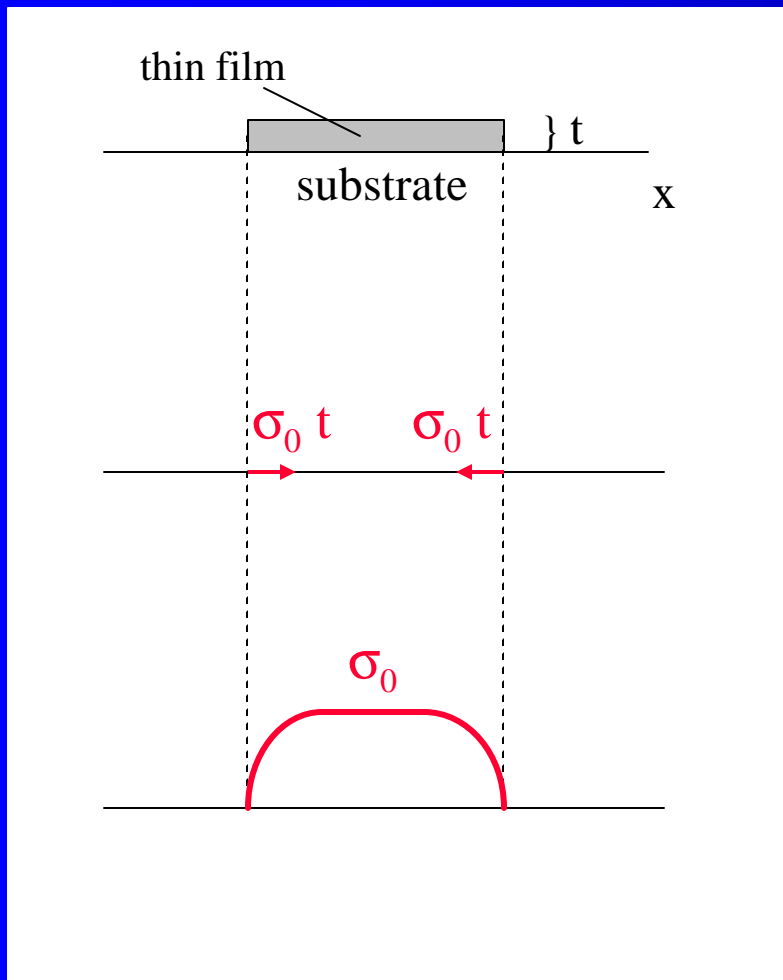
Free surfaces cannot support normal stress ( $\sigma_{xx} n_x = 0$ )

➤ assess the effect of feature width on in-plane normal stress ( $\sigma_{xx}$ )

Measure out-of-plane lattice deformation to determine in-plane stress

- assume  $\sigma_{zz} = 0$ ,  $\sigma_{yy} = \sigma_0$  (stress in blanket film)

# Mechanical modeling



Elastic half-space solutions

- substrate is semi-infinite

Edge-force model

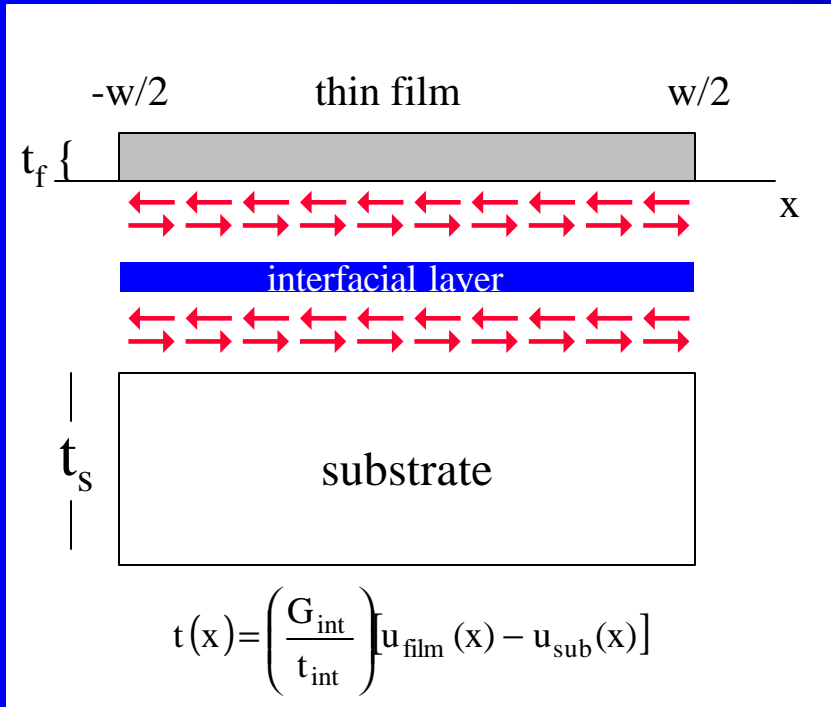
- Blech and Meieran (based on Love)
- interaction at film edges

Distributed-force model

- Hu
- decay in normal stress dictated by compatibility at interface



# Mechanical modeling (cont.)



Finite-thickness formulations

- elastic load transfer through shear across interface
- film and substrate possess equal widths ( $w$ )

Lap shear

- Suhir
- eigenvalue,  $K = f(E_i, t_i)$

Shear Lag

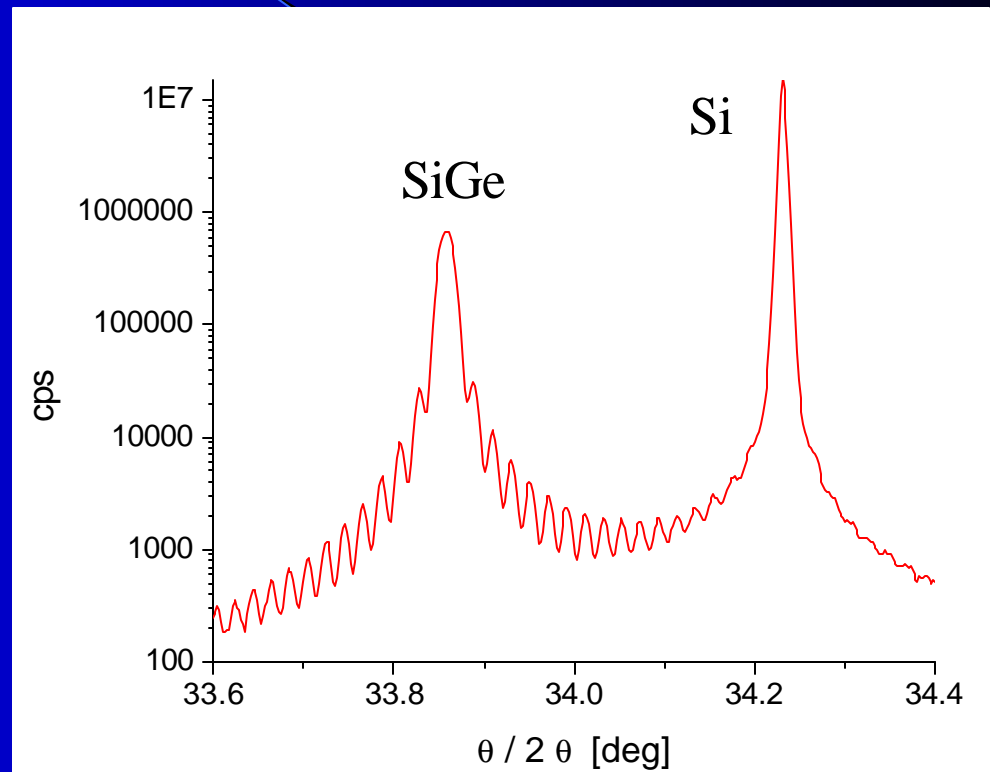
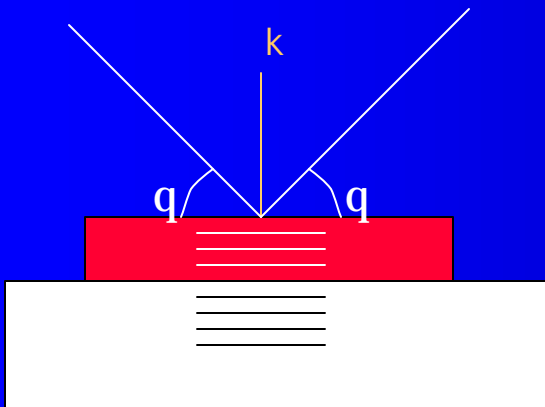
- Chen and Nelson
- shear is controlled by interfacial compliance parameter ( $G_{int}/t_{int}$ )

As feature width becomes infinite ( $w \rightarrow \infty$ ), results asymptote to Timoshenko model

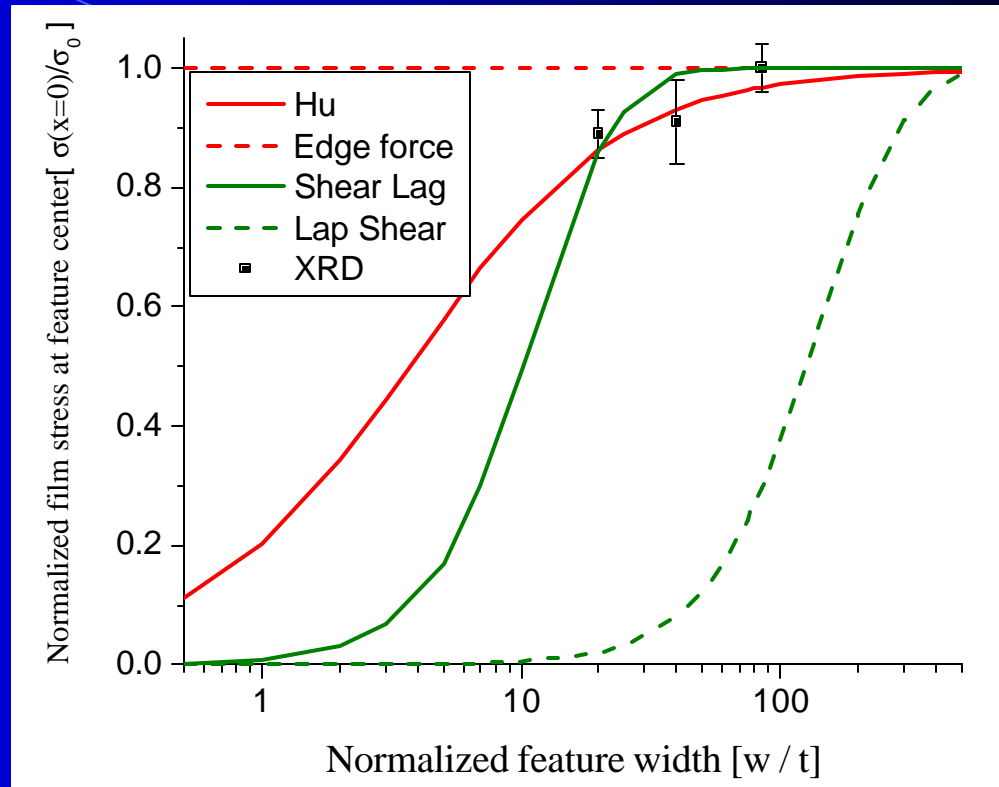
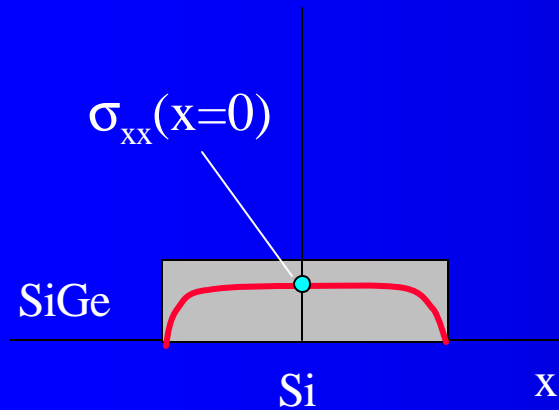
# Measurements

blanket SiGe prior to etching

- $\theta / 2\theta$  scans at feature centers
- Difference in Si (004) and SiGe (004) peak position
  - out-of-plane SiGe strain
  - normal stress at feature center



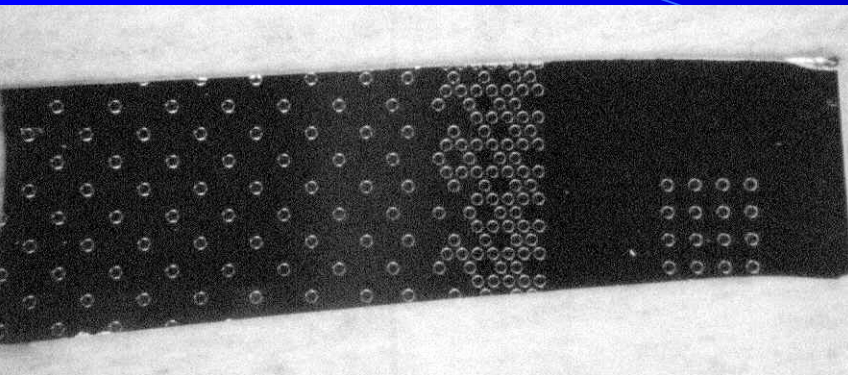
# Comparison of stress measurements to models



- Elastic relaxation in SiGe features on Si due to edge effects:
  - close to Hu and shear lag approximations
- More comprehensive models are being developed to incorporate:
  - out-of-plane elastic relaxation
  - observed strain decay in substrate outside of feature

# High-Resolution Microdiffraction

- Full reciprocal space mapping of single-crystal reflections.
- Necessary to resolve the epitaxial strain effects.
- Requires a parallel beam and analyzer crystal.
- Requires some optical advances.



Optical micrograph.

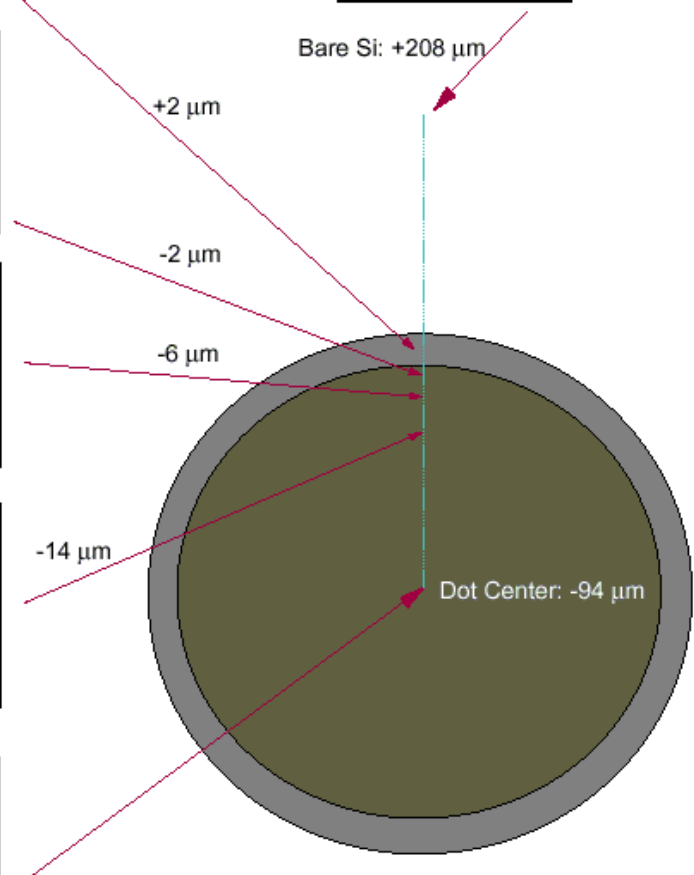
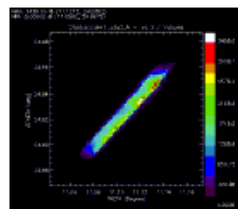
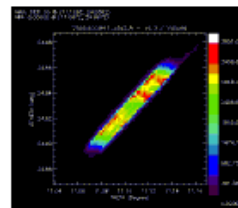
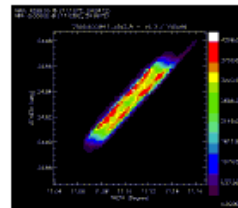
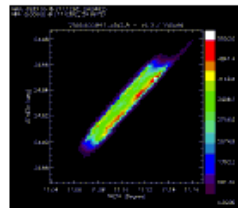
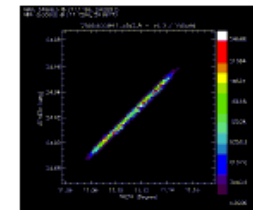
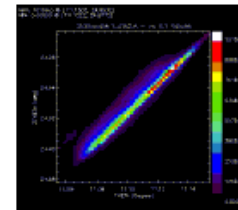
We observe the formation of a second peak.

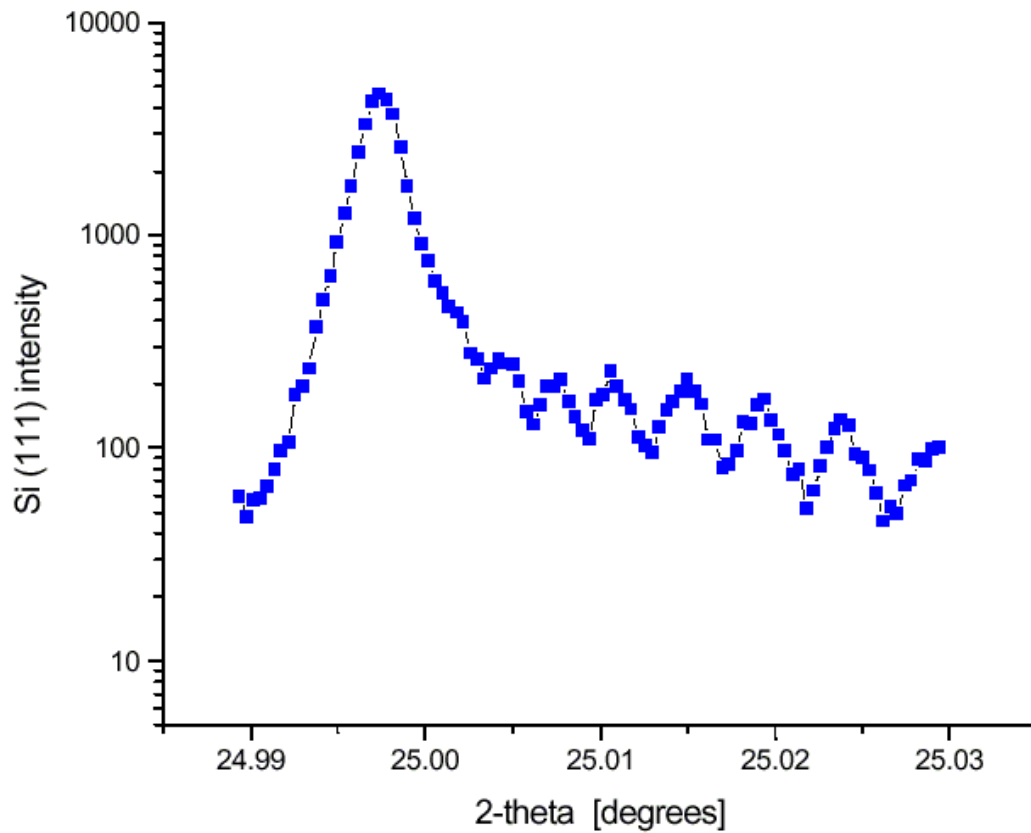
We also observe some Kiessig fringes.



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Reciprocal Space Maps of Si (111) diffraction  
190  $\mu\text{m}$  diameter Ni dots (1  $\mu\text{m}$  thick) on Si (111)



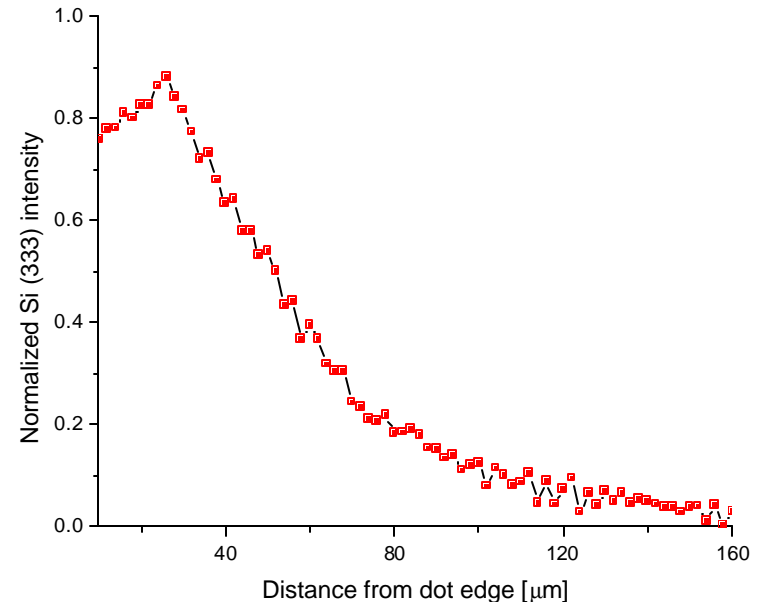
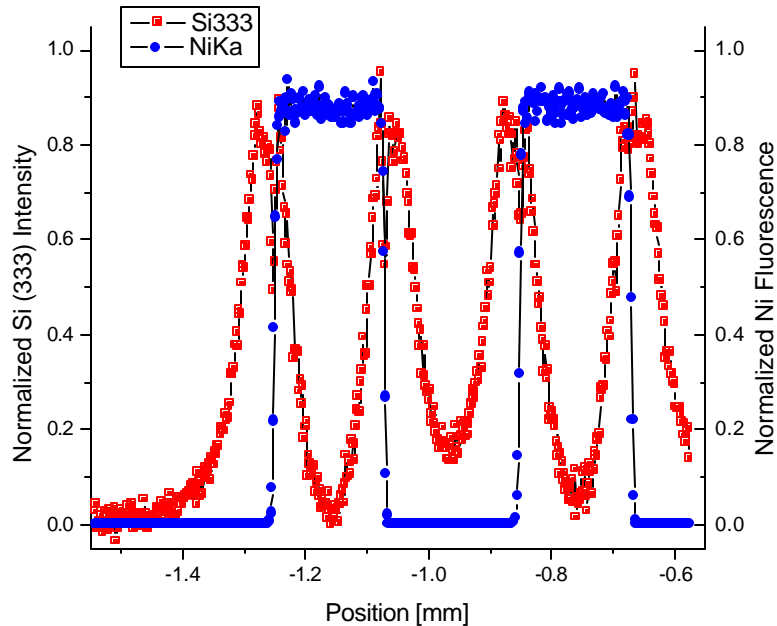


# Summary and future work

- X-ray microbeam measurements reveal strain in thin film / substrate systems
- Extent of strain fields in substrate
  - more than 100 times feature thickness away from edge
  - not predicted by current mechanical models
    - dynamic diffraction (H. Yan)
- Edge effects in thin film features
  - elastic relaxation measured in SiGe stripes
- Mechanical modeling implemented to describe observed behavior
  - analytical, FEM (S. Polvino)

# Enhanced Si (333) intensity

- Line scans of Si (333) vs. position confirm diffracted intensity increase due to strain
- Effects of Ni dot observed in Si substrate approximately 120  $\mu\text{m}$  away





# Enhanced x-ray diffraction

- Maps of Ni K $\alpha$  fluorescence and Si (333) diffraction  
- effects of strain on dynamic to kinematic transition in Si single crystal substrate

